

Equilibration of isolated macroscopic quantum systems

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Abstract. We investigate the equilibration of an isolated macroscopic quantum system in the sense that deviations from a steady state become unmeasurably small for the overwhelming majority of times within any sufficiently large time interval. The main requirements are that the initial state, possibly far from equilibrium, exhibits a macroscopic population of at most one energy level and that degeneracies of energy eigenvalues and of energy gaps (differences of energy eigenvalues) are not of exceedingly large multiplicities. Our approach closely follows and extends recent works by Short and Farrelly [2012 New J. Phys. **14** 013063], in particular going beyond the realm of finite-dimensional systems and large effective dimensions.

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1. Introduction

It is a basic everyday experience that isolated macroscopic systems, i.e. systems consisting of many particles or other microscopic degrees of freedom, approach some steady equilibrium state after a sufficiently long time evolution, no matter how far from equilibrium they started out. More precisely, for every single run of the experiment, one still may encounter certain statistical or quantum mechanical fluctuations, especially for microscopic observables, but on the average over many repetitions of the experiment, all expectation values appear to equilibrate.

The reconciliation of this irreversible behavior with quantum mechanical reversibility and revival/recurrence properties is a long standing problem [1] which has recently be reconsidered from a new viewpoint, without focusing on any specific model class and without any modification/approximation of the exact quantum mechanical time evolution [2–7]. The key point of these works is to show that the expectation values may still exhibit everlasting small fluctuations around their equilibrium values, as well as very rare large excursions away from equilibrium (including the above-mentioned recurrences), but quantitatively these fluctuations are either unobservably

small compared to any reasonably achievable resolution limit, or exceedingly rare on any realistic time scale after initial transients have died out. In this sense, the system indeed equilibrates.

Originally, these conclusions have been based on the following main assumptions [2–5]:

- (i) The considered observables represent experimental measurement devices with a finite instrumental range and a possibly very small but still ‘reasonable’ resolution limit.
- (ii) The initial condition exhibits a small occupation probability of every single energy level, which is very plausible in view of the unimaginably large level density of typical macroscopic systems.
- (iii) All energy eigenvalues are non-degenerate.
- (iv) All energy gaps are non-degenerate, i.e. a pair of distinct energy eigenvalues never exhibits the same energy difference as some other pair.
- (v) Either the considered Hilbert space must be finite-dimensional [3, 4], or some formal manipulations are not rigorously justified [2, 5], in particular interchanging the limit of infinite dimensions with the long-time limit.

The restrictions (iii) and (iv) have recently been overcome in two very important contributions by Short [6] and by Short and Farrelly [7]. In our present work, we closely follow and further extend their approach by relaxing also the above conditions (ii) and (v). Namely, we only require that the second largest level population must be small, while the occupation probability of one level may be macroscopic (non-small). Such a case may e.g. be of relevance for thermal equilibrium states at extremely low temperatures. Furthermore, we will admit and treat with care (countably) infinite dimensional systems.

Our present approach also bears resemblance to recent advancements made by Goldstein and coworkers of ideas originally due to von Neumann [8–11]. The main difference is that in these works an alternative notion is adopted of when a system is in or close to equilibrium, and the main emphasis is laid on macroscopic (coarse-grained) observables, exhibiting the same expectation value for most states within any quantum mechanical energy shell.

Furthermore, our approach is complementary to numerous recent investigations of equilibration for various specific systems, observables, and initial conditions, and often with a main focus on the role of (non-)integrability, see e.g. [12–28] and references therein.

Another issue closely related to equilibration is the problem of thermalization, i.e., the question whether, and to what extent, the above mentioned equilibrium states agree with any one of Gibbs’s statistical ensembles. This important issue, either for an isolated system *per se* or for an isolated system-plus-bath composite, has been recently addressed in e.g., [2–5, 8–24, 29, 30], but will not be considered here in any further detail. In other words, our notion of *equilibrium* is weaker than that of *thermal equilibrium*.

2. General Framework

2.1. System and Hamiltonian

We consider an isolated system, confined to a finite region of space and involving a finite number of particles. Later we will mainly be interested in macroscopic systems, but for the moment any finite number of degrees of freedom is admitted. In particular, we may be dealing with a compound system, consisting of a subsystem of actual interest and its environment (reservoir or thermal bath).

According to standard quantum mechanics, such a system is modeled by a time-independent Hamiltonian H on a separable (i.e. at most countably infinite-dimensional) Hilbert space \mathcal{H} . Since we consider the system to be confined to a finite region of space, all eigenvectors of H represent bound states and the spectrum of H is discrete (pure point). As a consequence, the Hamiltonian can be written in the form

$$H = \sum_n E_n P_n, \quad (1)$$

where the P_n are projectors onto the eigenspaces of H with eigenvalues E_n , satisfying

$$P_m P_n = \delta_{mn} P_n, \quad (2)$$

$$\sum_n P_n = 1, \quad (3)$$

$$E_n \neq E_m \quad \text{if } n \neq m. \quad (4)$$

Here, $n, m \in \{1, \dots, d_E\}$, where the number d_E of distinct energy eigenvalues may be finite or infinite. The symbol \sum_n indicates a summation over all those n -values, δ_{mn} is the Kronecker symbol, and 1 the identity on \mathcal{H} . In particular, any energy eigenvalue E_n is allowed to be degenerate and its multiplicity is given by

$$\mu_n := \text{Tr}\{P_n\}, \quad (5)$$

where Tr denotes the trace on \mathcal{H} . The dimension of \mathcal{H} thus amounts to $\sum_n \mu_n$ and may be finite or infinite.

2.2. States and dynamics

The system's state at time t is captured as usual by a density operator $\rho(t)$, describing either a statistical ensemble (mixed state) or a pure state, and evolving in time according to $\rho(t) = U_t \rho(0) U_t^\dagger$ with time-evolution operator $U_t := \exp\{-iHt\}$ and $\hbar = 1$. With (1) we can conclude that

$$\rho(t) = \sum_{mn} \rho_{mn}(0) \exp[-i(E_m - E_n)t], \quad (6)$$

where we have introduced the auxiliary operators

$$\rho_{mn}(t) := P_m \rho(t) P_n. \quad (7)$$

While $\rho_{nn}(t)$ are thus time-independent and self-adjoint operators, the same generically does not hold for $\rho_{mn}(t)$ when $m \neq n$. In particular, $\rho_{nn}(t)$ equals $\rho_{nn}(0)$ and the time-argument will often be omitted.

2.3. Realistic observables

Observables are represented as usual by self-adjoint operators A with expectation values $\text{Tr}\{\rho(t)A\}$. In order to model real experimental measurements it is however not necessary to admit any arbitrary self-adjoint operator [31–38]. Rather, it is sufficient to focus on *realistic observables* in the following sense [2, 5, 39]: Any observable A must represent an experimental device with a *finite range* of possible outcomes of a measurement,

$$\Delta_A := \sup_{\psi \in S(\mathcal{H})} \langle \psi | A | \psi \rangle - \inf_{\psi \in S(\mathcal{H})} \langle \psi | A | \psi \rangle = a_{\text{sup}} - a_{\text{inf}} < \infty, \quad (8)$$

where

$$S(\mathcal{H}) := \{\psi \in \mathcal{H} \mid \langle \psi | \psi \rangle = 1\} \subset \mathcal{H} \quad (9)$$

denotes the set of normalized vectors in \mathcal{H} . Moreover, this working range Δ_A of the device must be limited to experimentally reasonable values compared to its *resolution limit* δA . All measurements known to the present authors yield less than 20 relevant digits, i.e.

$$\Delta_A / \delta A \leq 10^{20}. \quad (10)$$

Maybe some day 100 or 1000 relevant digits will become feasible, but it seems reasonable that a theory which does not go very much beyond that will do. Note that similar restrictions also apply to ‘numerical experiments’ by computer simulations.

According to (8), all eigenvalues of A must be contained within the finite interval $[a_{\text{inf}}, a_{\text{sup}}]$ and the operator norm

$$\|A\| := \sup_{\psi \in S(\mathcal{H})} \|A|\psi\rangle\| \quad (11)$$

is finite and equal to $\max\{|a_{\text{inf}}|, |a_{\text{sup}}|\}$. (As usual, the vector norm on the right hand side of (11) is the one induced by the scalar product on \mathcal{H}).

2.4. Level populations

The specific observable $A = P_n$ describes the population of the energy level E_n with expectation value (occupation probability)

$$p_n := \text{Tr}\{P_n \rho(t)\} = \text{Tr}\{\rho_{nn}\}. \quad (12)$$

The last relation shows the time-independence of p_n and follows from (2), (7), and the invariance of the trace under cyclic permutations.

For a system with f degrees of freedom there are roughly $10^{O(f)}$ energy eigenstates with eigenvalues in every interval of 1J beyond the ground state energy ([40]; for a more detailed discussion, see also section 2.1 of [5]). The same estimate carries over to the number of energy eigenvalues under the assumption that their multiplicities (5) are much smaller than $10^{O(f)}$. For a macroscopic system with $f = O(10^{23})$, the energy levels are thus unimaginably dense on any decent energy scale and even the most

careful experimentalist will not be able to populate only a few of them with significant probabilities p_n .

We recall that $\rho(t)$ may be a pure state, but the case of foremost interest is on mixed states describing a statistical ensemble. Then, p_n describes an ensemble average over many repetitions of the experiment. Hence, an ‘accidentally large’ population of a few levels in one particular experimental run is still admissible, but very unlikely to occur again when the experiment is repeated.

To obtain a rough estimate, we imagine that there are exactly $10^{(10^{23})}$ energy levels per J. Even if the experimentalist can prepare the energy of the system with a fantastically small uncertainty of $10^{-(10^{22})}$ J, there still remain $N := 10^{0.9 \times 10^{23}}$ energy levels which may be occupied with significant probabilities. If all of them are populated equally, we obtain $p_n = 1/N$ for N of the indices n , and $p_n = 0$ for all other n . If not all N levels are populated equally, but rather any p_n may assume arbitrary values between zero and $10^{(10^{22})}$ times the average population $1/N$, we still obtain $p_n \leq 10^{-0.8 \times 10^{23}}$. Returning to the general case, we can conclude [2, 5, 39] that even if the system’s energy is fixed up to an extremely small experimental uncertainty, and even if the energy levels are populated extremely unequally, we still expect that even the largest ensemble-averaged level population p_n will be extremely small and typically satisfy the rough estimate

$$\max_n p_n = 10^{-O(f)}. \quad (13)$$

2.5. Macroscopic population of one energy level

There is one physically significant situation in which the above arguments may become questionable. Namely, for an isolated macroscopic system which approaches a thermal equilibrium state with an extremely low temperature, it might be conceivable that the ground state energy exhibits a macroscopic population, i.e. the corresponding p_n is no longer extremely small. Hence, we should omit that specific p_n in the maximization (13), formally written as

$$\max'_n p_n = 10^{-O(f)}. \quad (14)$$

In other words, the prime indicates that the largest p_n is not included into the maximization and hence $\max'_n p_n$ represents the second largest level population.

Further situations resulting in a non-small population of one single level may be caused e.g. by certain ‘gaps’ in the energy spectrum or by one level with an extremely high multiplicity (5).

Note that the expected relations $p_n \geq 0$ and $\sum_n p_n = 1$ readily follow from (3), (12), and the fact that $\rho(t)$ is non-negative and of unit trace. We thus can conclude that the maxima $\max_n p_n$ and $\max'_n p_n$ indeed exists—as anticipated in (13) and (14)—and that $0 \leq \sum'_n p_n < 1$, where the prime in \sum'_n excludes the index n belonging to the maximal p_n . It follows that

$$\sum_n p_n^2 \leq \max'_n p_n \sum'_n p_n \leq \max'_n p_n, \quad (15)$$

$$\max'_n p_n = (\max'_n p_n^2)^{1/2} \leq (\sum'_n p_n^2)^{1/2}, \quad (16)$$

and we can conclude that

$$\max'_n p_n \text{ small} \Leftrightarrow \sum'_n p_n^2 \text{ small}. \quad (17)$$

In references [3, 4, 6, 7], the quantity $d_{\text{eff}} := 1/\sum_n p_n^2$, called the effective dimension of the state $\rho(t)$, is introduced. It quantifies the number of distinct energies that contribute notably to this state, and is required to be a large number. Observing that the equivalence (17) also applies without primes, we see that the requirement of a large effective dimension is fulfilled if and only if the maximal level population $\max_n p_n$ is small. However, in the more general case including the primes in (17), as considered in our present work, the effective dimension d_{eff} may not be large any more.

2.6. Equilibration and equilibrium ensemble

Generically, the statistical ensemble $\rho(t)$ is not stationary right from the beginning, in particular for an initial condition $\rho(0)$ out of equilibrium. But if the right hand side of (6) depends on t initially, it cannot approach for large t any time-independent ‘equilibrium ensemble’ whatsoever. In fact, any mixed state $\rho(t)$ returns arbitrarily close (with respect to some suitable distance measure in Hilbert space) to its initial state $\rho(0)$ for certain, sufficiently large times t , as demonstrated for instance in appendix D of [41].

We will therefore focus on the weaker notion of equilibration outlined in section 1, requiring the existence of a time-independent ‘equilibrium state’ ω (density operator) with the property that the difference

$$\sigma(t) := \text{Tr}\{\rho(t)A\} - \text{Tr}\{\omega A\} \quad (18)$$

between the true expectation value $\text{Tr}\{\rho(t)A\}$ and the equilibrium reference value $\text{Tr}\{\omega A\}$ is unresolvably small for the overwhelming majority of times t contained in any sufficiently large (but finite) time interval $[0, T]$. (Note that initial transients become irrelevant if T is chosen large enough.)

Heuristically, if any such equilibrium ensemble exists, then it should be given by the infinite time average of $\rho(t)$. In view of (6) this suggests the definition

$$\omega := \sum_n \rho_{nn}. \quad (19)$$

However, from a more rigorous viewpoint, it is not so obvious that averaging (6) over arbitrary but finite times leads to a well-defined long-time limit, which is furthermore given by (19). Specifically, for infinite-dimensional systems, interchanging the infinite time limit with the infinite double-sum in (6) is problematic. We avoid all these difficulties by defining ω according to (19) without any reference to averages over time. An alternative and entirely unproblematic viewpoint is to consider ω as the time-independent part of $\rho(t)$.

One readily sees that ω inherits from $\rho(t)$ the properties of being self-adjoint, non-negative, and of unit trace. Furthermore, ω satisfies the trivial time evolution $U_t \omega U_t^\dagger = \omega$. In other words, ω is indeed a perfectly well-defined density operator.

We finally note that, as far as the differences in (18) are concerned, nothing changes if A is replaced by $A + c1$ with an arbitrary real c . Thus, we henceforth can assume without loss of generality that $a_{\sup} = -a_{\inf}$ in (8), implying with (11) that

$$\|A\| = \Delta_A/2. \quad (20)$$

3. From infinite to finite dimensions

We focus on infinite-dimensional Hilbert spaces \mathcal{H} and denote the normalized eigenvectors of the Hamiltonian H by $|\nu\rangle$ with $\nu = 1, 2, \dots$. For any given positive integer d we define the projectors

$$P := \sum_{\nu=1}^d |\nu\rangle\langle\nu|, \quad (21)$$

$$Q := 1 - P. \quad (22)$$

For an arbitrary density operator ρ and any observable A it follows that

$$\text{Tr}\{\rho A\} = \text{Tr}\{(P + Q)\rho(P + Q)A\} = R_1 + R_2 + R_3 \quad (23)$$

with

$$R_1 := \text{Tr}\{P\rho PA\}, \quad (24)$$

$$R_2 := \text{Tr}\{Q\rho A\}, \quad (25)$$

$$R_3 := \text{Tr}\{P\rho QA\}. \quad (26)$$

Making use of $P^2 = P$ and the cyclic invariance of the trace, one can rewrite R_1 as $\text{Tr}\{(P\rho P)(PAP)\}$ or

$$R_1 = \text{Tr}\{\tilde{\rho}\tilde{A}\}, \quad (27)$$

$$\tilde{\rho} := P\rho P, \quad (28)$$

$$\tilde{A} := PAP. \quad (29)$$

To further evaluate R_2 we represent the self-adjoint operator ρ in terms of its eigenvalues ρ_ν and eigenvectors $|\phi_\nu\rangle$,

$$\rho = \sum_{\nu=1}^{\infty} \rho_\nu |\phi_\nu\rangle\langle\phi_\nu|. \quad (30)$$

Since ρ is non-negative, all ρ_ν are non-negative and

$$\rho^{1/2} := \sum_{\nu=1}^{\infty} \sqrt{\rho_\nu} |\phi_\nu\rangle\langle\phi_\nu| \quad (31)$$

is a well-defined, self-adjoint operator with the property that $\rho^{1/2}\rho^{1/2} = \rho$. It follows that

$$|R_2|^2 = |\text{Tr}\{(Q\rho^{1/2})(\rho^{1/2}A)\}|^2 \leq \text{Tr}\{Q\rho Q\} \text{Tr}\{A\rho A\}, \quad (32)$$

where we exploited the Cauchy–Schwarz inequality

$$|\mathrm{Tr}\{B^\dagger C\}|^2 \leq \mathrm{Tr}\{B^\dagger B\} \mathrm{Tr}\{C^\dagger C\} \quad (33)$$

for the scalar product $\mathrm{Tr}\{B^\dagger C\}$ of arbitrary operators B and C (for which all traces in (33) exist). The last term in (32) equals $\mathrm{Tr}\{\rho A^2\}$, and by evaluating the trace by means of the orthonormal basis $|\phi_n\rangle$ one can infer with (11) and (30) that

$$\mathrm{Tr}\{\rho A^2\} \leq \|A^2\| \mathrm{Tr}\{\rho\} \leq \|A\|^2, \quad (34)$$

where we exploited that $\mathrm{Tr}\{\rho\} = 1$ and $\|A^2\| = \|A\|^2$ in the last relation. Finally, we conclude from (21) and (22) that

$$\mathrm{Tr}\{Q\rho Q\} = \sum_{\nu=d+1}^{\infty} \langle \nu | \rho | \nu \rangle \quad (35)$$

and hence

$$|R_2|^2 \leq \|A\|^2 \sum_{\nu=d+1}^{\infty} \langle \nu | \rho | \nu \rangle. \quad (36)$$

Next, starting from (26), we rewrite R_3 as $\mathrm{Tr}\{AP\rho Q\}$. Noting that all four operators under this trace are self-adjoint and that $\mathrm{Tr}\{B^\dagger\} = \mathrm{Tr}\{B\}^*$ for arbitrary operators B , we can conclude that $|R_3| = |\mathrm{Tr}\{Q\rho PA\}|$. Proceeding similarly as in (32)–(34) and using $\mathrm{Tr}\{\tilde{\rho}\} \leq 1$ one finds that

$$|R_3|^2 \leq \mathrm{Tr}\{Q\rho Q\} \|A\|^2 \mathrm{Tr}\{\tilde{\rho}\} \leq \|A\|^2 \sum_{\nu=d+1}^{\infty} \langle \nu | \rho | \nu \rangle. \quad (37)$$

This in turn implies via (23)–(29) that

$$|\mathrm{Tr}\{\rho A\} - \mathrm{Tr}\{\tilde{\rho} \tilde{A}\}| \leq 2\|A\| \left(\sum_{\nu=d+1}^{\infty} \langle \nu | \rho | \nu \rangle \right)^{1/2} \quad (38)$$

for arbitrary density operators ρ . Applying this relation to the specific density operators $\rho(t)$ in (6) and ω in (19) we obtain

$$|\mathrm{Tr}\{\rho(t)A\} - \mathrm{Tr}\{\omega A\}| = |\mathrm{Tr}\{\tilde{\rho}(t)\tilde{A}\} - \mathrm{Tr}\{\tilde{\omega}\tilde{A}\}| + R \quad (39)$$

with

$$R \leq |\mathrm{Tr}\{\rho(t)A\} - \mathrm{Tr}\{\omega A\} - \mathrm{Tr}\{\tilde{\rho}(t)\tilde{A}\} + \mathrm{Tr}\{\tilde{\omega}\tilde{A}\}| \quad (40)$$

$$\leq 4\|A\| \left(\sum_{\nu=d+1}^{\infty} \langle \nu | \rho(0) | \nu \rangle \right)^{1/2}. \quad (41)$$

In (40) we exploited the fact that $|x| - |y| \leq |x - y|$ for arbitrary real x and y , while in (41) we applied (38) to $\rho(t)$ and ω and we took into account that, according to (6) and (19), both $\langle \nu | \rho(t) | \nu \rangle$ and $\langle \nu | \omega | \nu \rangle$ are equal to $\langle \nu | \rho(0) | \nu \rangle$.

Observing that $\sum_{\nu=1}^d \langle \nu | \rho(0) | \nu \rangle$ increases with d and approaches $\mathrm{Tr}\{\rho(0)\} = 1$ for $d \rightarrow \infty$ it follows that, for any given $\epsilon > 0$, there exists a finite $d(\epsilon)$ with the property

that $R \leq \|A\|\epsilon$. According to (10), upon choosing $\epsilon = 10^{-20}$ and observing (20), we can conclude that

$$R \leq \delta A/2 \quad (42)$$

with one common, finite d for all experimentally realistic observables A .

As far as experimentally resolvable differences (18) are concerned, it thus follows from (39) and (42) that it is sufficient to consider, instead of $\rho(t)$ and A , their counterparts $\tilde{\rho}(t)$ and \tilde{A} . According to (20), (28) and (29) these are the projections/restrictions of the original operators $\rho(t)$ and A onto the finite dimensional sub-Hilbert space $\tilde{\mathcal{H}} \subset \mathcal{H}$, spanned by the first d energy eigenvectors $\{|\nu\rangle\}_{\nu=1}^d$. Note that while $\tilde{\mathcal{H}}$ is independent of A , it does depend on $\rho(0)$ and H in general.

It remains to be shown that the entire framework set out in section 2 can be consistently restricted to the finite-dimensional Hilbert space $\tilde{\mathcal{H}}$: Observing that the projectors P_n from (1) commute with the projector P defined in (21) implies that

$$\tilde{P}_n := PP_nP = PP_n = P_nP. \quad (43)$$

Setting $\tilde{H} := PHP$ and keeping only indices n with non-zero \tilde{P}_n , relations (1)–(5) remain valid, but now with finite sums \sum_n and finite multiplicities $\tilde{\mu}_n$. Furthermore, one sees that \tilde{H} indeed reproduces the correct time evolution of $\tilde{\rho}(t)$ with finite sums in (6). While $\tilde{\rho}(t)$ is still non-negative and self-adjoint, the trace now satisfies

$$\text{Tr}\{\tilde{\rho}(t)\} = \sum_n \tilde{p}_n \leq 1. \quad (44)$$

Likewise, with respect to the operator norm (11) and the level population (12) one finds that

$$\|\tilde{A}\| \leq \|A\|, \quad \tilde{p}_n \leq p_n. \quad (45)$$

4. Finite-dimensional systems

The main objective of this section is to establish bounds on the difference

$$\tilde{\sigma}(t) := \text{Tr}\{\tilde{\rho}(t)\tilde{A}\} - \text{Tr}\{\tilde{\omega}\tilde{A}\}, \quad (46)$$

where tildes indicate the projections/restrictions to the finite-dimensional Hilbert space $\tilde{\mathcal{H}}$ from the previous subsection in case the original Hilbert space \mathcal{H} was infinite-dimensional (otherwise the tildes are redundant). We recall that $d < \infty$ denotes the dimension of $\tilde{\mathcal{H}}$ (see below (42)) and $\tilde{d}_E \leq d$ the number of distinct energy eigenvalues E_n of \tilde{H} (see below (4)).

Adopting the approach of Short and Farrelly [7], we start by considering the quantity $\langle \tilde{\sigma}^2(t) \rangle_T$, where $\langle \cdot \rangle_T$ denotes a temporal average over the time interval $[0, T]$ with arbitrary but finite $T > 0$. From (6) and (19) we can infer that

$$\langle \tilde{\sigma}^2(t) \rangle_T = \left\langle \left| \sum_{m \neq n} \text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\} \exp[-i(E_m - E_n)t] \right|^2 \right\rangle_T, \quad (47)$$

where $\tilde{\rho}_{mn}(0)$ is abbreviated as $\tilde{\rho}_{mn}$ and the sum runs over the finite set of pairs of labels

$$\mathcal{G} := \{(m, n) \mid m, n \in [1, \dots, \tilde{d}_E], m \neq n\}. \quad (48)$$

For any $\alpha = (m, n) \in \mathcal{G}$ we define

$$G_\alpha := E_m - E_n, \quad v_\alpha := \text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\}. \quad (49)$$

We thus can rewrite (47) as

$$\langle \tilde{\sigma}^2(t) \rangle_T = \left\langle \left| \sum_{\alpha} v_{\alpha} \exp[-iG_{\alpha}t] \right|^2 \right\rangle_T = \sum_{\alpha, \beta} v_{\alpha}^* M_{\alpha\beta} v_{\beta}, \quad (50)$$

where we introduced the self-adjoint, non-negative, finite-dimensional matrix M with matrix elements

$$M_{\alpha\beta} := \langle \exp[i(G_{\alpha} - G_{\beta})t] \rangle_T. \quad (51)$$

Denoting by $\|M\|$ the standard operator norm of the matrix M (see (11)), it follows that [7]

$$\langle \tilde{\sigma}^2(t) \rangle_T \leq S \|M\| \quad (52)$$

$$S := \sum_{\alpha} |v_{\alpha}|^2 = \sum_{m \neq n} |\text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\}|^2. \quad (53)$$

Bounds on the two factors S and $\|M\|$ in (52) are constructed in the following two subsections.

4.1. Bound on S

We exploit (2), (7), and the cyclic invariance of the trace to conclude that

$$\text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\} = \text{Tr}\{\tilde{P}_m\tilde{\rho}\tilde{P}_n\tilde{A}\tilde{P}_m\}. \quad (54)$$

Similarly to the derivation in (30)–(32), we write

$$\tilde{P}_m\tilde{\rho}\tilde{P}_n\tilde{A}\tilde{P}_m = (\tilde{P}_m\tilde{\rho}^{1/2})(\tilde{\rho}^{1/2}\tilde{P}_n\tilde{A}\tilde{P}_m) \quad (55)$$

from which it follows that

$$|\text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\}|^2 \leq \tilde{p}_m \text{Tr}\{\tilde{\rho}_{nn}\tilde{A}\tilde{P}_m\tilde{A}\}. \quad (56)$$

We first evaluate by means of (56) all summands in (53) with $n = 1$,

$$\begin{aligned} S_{n=1} &\leq \sum_{m \geq 2} \tilde{p}_m \text{Tr}\{\tilde{\rho}_{11}\tilde{A}\tilde{P}_m\tilde{A}\} \\ &\leq \max_{n \geq 2} p_n \text{Tr}\left\{\tilde{\rho}_{11}\tilde{A} \sum_{m \geq 2} \tilde{P}_m\tilde{A}\right\} \\ &\leq \max_{n \geq 2} p_n \text{Tr}\{\tilde{\rho}_{11}\} \left\| \tilde{A} \sum_{m \geq 2} \tilde{P}_m\tilde{A} \right\| \\ &\leq \max_{n \geq 2} p_n \|A\|^2. \end{aligned} \quad (57)$$

In the second line we used that $\tilde{p}_m \leq p_m \leq \max_{n \geq 2} p_n$ for all $m \geq 2$, see (45). The third line is based on a similar line of reasoning as in (34), exploiting that $\tilde{\rho}_{11}$ is a

non-negative, self-adjoint operator. In the last line we used that $\text{Tr}\{\tilde{\rho}_{11}\} = \tilde{p}_1 \leq 1$ (see (12) and (44)), that $\|BC\| \leq \|B\|\|C\|$ for arbitrary operators B, C of finite norm, and that $\sum_{m \geq 2} \tilde{P}_m$ is a projector and hence of unit norm.

For symmetry reasons, the same estimate as in (57) applies for the summands with $m = 1$ in (53). The remaining summands in (53) satisfy $m \neq n$ and $m, n \geq 2$. By including also those with $m = n$, the sum can only increase, resulting in

$$S \leq 2\|A\|^2 \max'_n p_n + \sum'_{m,n} |\text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\}|^2, \quad (58)$$

where the prime indicates that indices 1 are excluded from the maximization and the summation. Clearly, instead of this special index 1 we could have selected any other index as well. Thus, in agreement with section 2.5, the prime can and will be understood as excluding the index belonging to the maximally populated level.

The remaining sum in (58) can be estimated by means of the two non-negative, self-adjoint operators

$$\tilde{\omega}' := \sum'_n \tilde{\rho}_{nn}, \quad \tilde{\omega}'' := \sum'_m \tilde{p}_m \tilde{P}_m \quad (59)$$

in the following way:

$$\begin{aligned} \sum'_{m,n} |\text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\}|^2 &\leq \text{Tr}\{\tilde{\omega}'\tilde{A}\tilde{\omega}''\tilde{A}\} \leq \sqrt{\text{Tr}\{(\tilde{\omega}')^2\tilde{A}^2\} \text{Tr}\{(\tilde{\omega}'')^2\tilde{A}^2\}} \\ &\leq \sqrt{\text{Tr}\{(\tilde{\omega}')^2\}\|\tilde{A}\|^2 \text{Tr}\{(\tilde{\omega}'')^2\}\|\tilde{A}\|^2} = \|\tilde{A}\|^2 \sqrt{\sum'_n \text{Tr}\{\tilde{\rho}_{nn}^2\} \sum'_m \tilde{\mu}_m \tilde{p}_m^2}. \end{aligned} \quad (60)$$

In the first inequality, we exploited (56), the next two ones follow by arguments similar to the ones in (32) and (34). The last equation is based on (2), (5), (7) and (59).

Once again, the line of reasoning in (60) follows very closely that of Short and Farrelly [6, 7]. The main difference is that these authors focus, in a first step, solely on pure states and only in the end extend their result to mixed states via purification. Along this line, one actually arrives at a final result which is slightly different from (60), namely

$$\sum'_{m,n} |\text{Tr}\{\tilde{\rho}_{mn}\tilde{A}\}|^2 \leq \|\tilde{A}\|^2 \sum'_n \tilde{p}_n^2. \quad (61)$$

Closer inspection shows that (60) and (61) agree if and only if all energies are non-degenerate. In any other case, one can show that the bound (61) is sharper than (60). On the other hand, one readily sees that $\text{Tr}\{\tilde{\rho}_{nn}^2\} \leq \tilde{p}_n^2$ and hence

$$\sqrt{\sum'_n \text{Tr}\{\tilde{\rho}_{nn}^2\} \sum'_m \tilde{\mu}_m \tilde{p}_m^2} \leq \max'_m \sqrt{\tilde{\mu}_m} \sum'_n \tilde{p}_n^2. \quad (62)$$

The equality sign applies whenever $\rho(t)$ is a pure state contained in the maximally degenerate energy eigenspace, in any other case the inequality sign applies. In conclusion, (61) outperforms (60) by at most a factor of $\max'_m \sqrt{\tilde{\mu}_m}$, i.e. the square root of the maximal energy degeneracy.

The purification argument [6, 7] behind (61) is mathematically very appealing (somewhat reminiscent of evaluating real integrals by ‘complexification’) but its physical content remains slightly mysterious. It is reassuring that one can get at least as far as (60) without this argument, but it is annoying that (61) could not be fully recovered.

Working with the stronger bound (61) by Short and Farrelly, the estimate (58) for S in combination with (15) and (45) takes on the simple form

$$S \leq 3 \|A\|^2 \max'_n p_n. \quad (63)$$

While the maximization so far includes only a finite number of indices n , this restriction can be readily released, as the maximum can only increase in this way. As in section 2.5, the last factor then represents the second largest level population of the original, possibly infinite-dimensional system.

4.2. Bound on $\|M\|$ in terms of energy gaps

The main idea is that, since M is a finite-dimensional matrix, its operator norm $\|M\|$ converges towards a well-defined limit as the averaging time T (see (47), (51)) tends to infinity. Hence, $\|M\|$ can be readily bounded from above for all sufficiently large (but finite) T .

Quantitatively, by setting out from the inequality

$$\|M\| \leq \max_{\beta} \sum_{\alpha} |M_{\alpha\beta}|, \quad (64)$$

Short and Farrelly [7] derived the estimate

$$\|M\| \leq N(\epsilon) \left(1 + \frac{8 \log_2 \tilde{d}_E}{\epsilon T} \right) \quad (65)$$

for arbitrary $\epsilon > 0$ and $T > 0$. Here, \tilde{d}_E is the number of distinct energy eigenvalues E_n (see below (46)) and

$$N(\epsilon) := \max_E |\{\alpha \in \mathcal{G} \mid G_{\alpha} \in [E, E + \epsilon)\}|. \quad (66)$$

According to (48) and (49), $N(\epsilon)$ is thus the maximum number of energy gaps $G_{\alpha} = E_m - E_n$ in any interval of size ϵ .

The main implication of this result can also be deduced directly from (64): since we are dealing with finite-dimensional systems, the *finite number* of all matrix elements $|M_{\alpha\beta}|$ in (51) with $G_{\alpha} \neq G_{\beta}$ can be *simultaneously* bounded by an arbitrarily small upper limit for sufficiently large T . Hence, their contribution to (64) can be made smaller than the contribution of all the remaining summands, satisfying $G_{\alpha} = G_{\beta}$ and thus $M_{\alpha\beta} = 1$. It follows for all sufficiently large T that

$$\|M\| \leq 2g, \quad (67)$$

where

$$g := \max_{\beta} |\{\alpha \in \mathcal{G} \mid G_{\alpha} = G_{\beta}\}| \quad (68)$$

denotes the maximal degeneracy of energy gaps. Note that only the energy eigenvalues E_n of the restricted, finite-dimensional Hamiltonian \tilde{H} contribute to \mathcal{G} in (48) and hence to the degenerate energy gaps counted in (68).

4.3. Problems in the infinite-dimensional limit

So far, we have assumed a finite dimensionality d of the Hilbert space $\tilde{\mathcal{H}}$. In this subsection we argue that it is intuitively suggestive that everything ‘should go well’ upon letting d go to infinity, but that a more rigorous justification is problematic. From the latter viewpoint, the considerations in section 3 are thus indispensable for infinite-dimensional systems.

First of all, since A has a finite range Δ_A , see (8), it follows that $\sigma(t)$ from (18) is contained in the finite interval $[-2\Delta_A, 2\Delta_A]$ for all times t . This suggest (but does not prove) that the temporal average $\langle \sigma^2(t) \rangle_T$ converges in the limit $T \rightarrow \infty$ even for infinite dimensional systems: although one can readily construct mathematical examples of bounded functions without a well-defined infinite-time average, it appears plausible that ‘reasonable’ physical models will result in functions $\sigma^2(t)$ which do not exhibit the pathologies of those examples.

On the other hand, for any given finite dimension d , equation (50) has a well defined $T \rightarrow \infty$ limit. Focusing on the simplest case of non-degenerate energy gaps, $M_{\alpha\beta}$ in (51) approaches $\delta_{\alpha\beta}$ and hence the inequality (52) turns into an equality with $\|M\| = 1$. Since S in (53) is positive and bounded by the d -independent estimate (63), it is once again suggestive that S itself converges for $d \rightarrow \infty$. Under the further assumption that the two limits $T \rightarrow \infty$ and $d \rightarrow \infty$ commute, one then readily finds an upper bound analogous to (69) for infinite dimensions and all sufficiently large, but finite, T .

Although these heuristic arguments appear plausible at first glance, some subtle open questions remain upon closer inspection: For infinite-dimensional systems one typically expects the existence of arbitrarily small, but non-vanishing energy gap differences $G_\alpha - G_\beta$. While each single matrix element (51) then still converges for $T \rightarrow \infty$, the same is no longer clear for the entire, infinite-dimensional matrix M and/or its norm $\|M\|$. For the same reason, $N(\epsilon)$ from (66) is expected to diverge for $d \rightarrow \infty$ and any fixed $\epsilon > 0$, so that (65) becomes useless. Likewise, our derivation of (67) breaks down. In other words, interchanging the limits $T \rightarrow \infty$ and $d \rightarrow \infty$ is a rather delicate, unsettled issue.

5. Main result and discussion

Combining (20), (52), (63) and (67), we obtain the inequality

$$\langle \tilde{\sigma}^2(t) \rangle_T \leq \frac{3}{2} g \Delta_A^2 \max'_n p_n \quad (69)$$

for all sufficiently large T .

For any given $\epsilon > 0$ and $T > 0$ we define the measure of all times $t \in [0, T]$ for which $|\tilde{\sigma}(t)| \geq \epsilon$ holds true,

$$\tilde{T}_\epsilon := \lambda(\{t \mid t \in [0, T] \text{ and } |\tilde{\sigma}(t)| \geq \epsilon\}), \quad (70)$$

where λ denotes the Lebesgue measure. It follows that $\tilde{\sigma}^2(t) \geq \epsilon^2$ for a set of times t of measure \tilde{T}_ϵ and $\tilde{\sigma}^2(t) \geq 0$ for all remaining times t in $[0, T]$. Hence the temporal average of $\tilde{\sigma}^2(t)$ over the time interval $[0, T]$ must be at least $\epsilon^2 \tilde{T}_\epsilon / T$,

$$\langle \tilde{\sigma}^2(t) \rangle_T \geq \frac{\epsilon^2 \tilde{T}_\epsilon}{T}. \quad (71)$$

Choosing $\epsilon = \delta A/2$, we can conclude from (69) and (71) that

$$\frac{\tilde{T}_{\delta A/2}}{T} \leq 6g \left(\frac{\Delta_A}{\delta A} \right)^2 \max'_n p_n \quad (72)$$

for all sufficiently large T .

Next we infer from (39), (42) and (46) that

$$|\text{Tr}\{\rho(t)A\} - \text{Tr}\{\omega A\}| \leq |\tilde{\sigma}(t)| + \frac{\delta A}{2}. \quad (73)$$

Analogously to (70), we define the measure of all times $t \in [0, T]$ with the property that $|\text{Tr}\{\rho(t)A\} - \text{Tr}\{\omega A\}|$ exceeds the experimental resolution limit δA ,

$$T_{\delta A} := \lambda(\{t \mid t \in [0, T] \text{ and } |\text{Tr}\{\rho(t)A\} - \text{Tr}\{\omega A\}| \geq \delta A\}). \quad (74)$$

In view of (70) with $\epsilon = \delta A/2$ and (73), we conclude that $T_{\delta A} \leq \tilde{T}_{\delta A/2}$. With (72) we thus arrive at the main result of our present work,

$$\frac{T_{\delta A}}{T} \leq 6g \left(\frac{\Delta_A}{\delta A} \right)^2 \max'_n p_n \quad (75)$$

for all sufficiently large T .

The left hand side of (75) represents the fraction of all times $t \in [0, T]$ for which there is an experimentally resolvable difference between the true expectation value $\text{Tr}\{\rho(t)A\}$ and the time-independent ‘equilibrium expectation value’ $\text{Tr}\{\omega A\}$.

On the right hand side, g is the maximal degeneracy of energy gaps from (68), i.e. the maximal number of (exactly) coinciding energy differences among all possible pairs of distinct energy eigenvalues of the reduced, finite-dimensional Hamiltonian \tilde{H} from section 3, and as such is determined by properties of both the Hamiltonian H and the initial condition $\rho(0)$. Alternatively, one may also take into account all energies of the full system Hamiltonian H , since the maximum can only increase in this way, but this increase might possibly become prohibitively huge for infinite dimensional systems (see also section 6).

The next factor $\Delta_A/\delta A$ appearing in (75) is the range-to-resolution ratio of A from section 2.3, i.e. a characteristic property of the observable A only, and can be considered as bounded according to (10) for all experimentally realistic measurements A . Going back to section 4.1, one readily sees that one could as well replace Δ_A by the range of the reduced observable \tilde{A} . This range typically is somewhat smaller than the original range Δ_A of A (see (45)), but this gain might often not be worth the effort.

Finally, $\max_n' p_n$ in (75) stands for the second-largest, ensemble-averaged occupation probability of the (possibly degenerate) energy eigenvalues E_n , see sections 2.4 and 2.5. Similarly as for A , one alternatively could maximize over the reduced level populations \tilde{p}_n , but often this will not be worthwhile. Essentially, $\max_n' p_n$ is thus a characteristic property of the initial condition $\rho(0)$, but obviously also the Hamiltonian H itself matters. Typically, one expects that the rough upper bound (14) applies, except if certain energy eigenvalues are so extremely highly degenerate that the multiplicities defined in (5) severely reduce the pertinent energy level density compared to the non-degenerate case, see section 2.4.

For a system with sufficiently many degrees of freedom f and no exceedingly large degeneracy of the energy eigenvalues and the energy gaps, we thus can conclude from (75) with (10) and (14) that the system behaves in every possible experiment exactly as if it were in the equilibrium state ω for the overwhelming majority of times within any sufficiently large (but finite) time interval $[0, T]$. In particular, T must obviously be much larger than the relaxation time in case of a far-from-equilibrium initial condition $\rho(0)$. A more detailed quantitative bound on T follows from the result (65) by Short and Farrelly [7].

We emphasize that even in the absence of any measurable difference between $\rho(t)$ and ω , the equilibrium state ω itself is never realized in the actual system, and as such is a purely formal, theoretical construct. In particular, the difference between $\text{Tr}\{\rho(t)A\}$ and $\text{Tr}\{\omega A\}$ is not a quantity one can measure in a real system, not even in principle.

Further interesting physical implications of (75) are discussed, in e.g., [5].

6. Conclusions

To summarize, by adopting and extending recent works by Short [6] and by Short and Farrelly [7], we demonstrated equilibration of isolated macroscopic quantum systems in the sense that deviations from a time-independent steady state are unmeasurably small for the overwhelming majority of times within any sufficiently large time interval. This conclusion applies for arbitrary systems with (countably) infinite dimensions, initial states exhibiting a macroscopic population of at most one energy level, and Hamiltonians without exceedingly large degeneracies of energy eigenvalues and energy gaps.

As soon as a model includes at least one continuous degree of freedom (e.g. a spatial coordinate), the pertinent Hilbert space is necessarily of infinite dimension. If the system is furthermore of finite spatial extension (e.g. due to confining walls), the Hamiltonian H features a discrete spectrum and can be written in the form (1). Both conditions are clearly satisfied in almost any model which is not based on some extreme simplifications. Moreover, it is practically impossible to prepare a real system so that only a finite number of energy eigenstates is populated. Rather, generically an infinite number of them contributes with possibly small, yet finite, amplitudes. Reducing or truncating this situation in whatever way to finite dimensions is especially problematic with respect to rigorous statements about the exact quantum mechanical evolution

over arbitrarily long time intervals. More precisely, interchanging the limit of infinite dimensions with the long time limit, as discussed in section 4.3, is a subtle problem, justifying the detailed treatment of the infinite-dimensional case in section 3.

Admitting systems with degenerate energy eigenvalues and energy gaps are among the most important steps forward achieved in [6, 7]. On the other hand, it is generally taken for granted that such degeneracies are absent in generic Hamiltonians, see e.g. [2, 3, 5, 12, 13, 42] and, in particular, section 3.2.1 of [43] and references therein. Roughly speaking, Hamiltonians with such degeneracies are of measure zero compared to ‘all’ Hamiltonians. They only arise in the presence of special reasons like (perfect) symmetries, additional conserved quantities, or fine-tuning of parameters, which can be ruled out for typical real systems provided they cannot be further decomposed into non-interacting subsystems [3]. It is reassuring that even some of those exceptions—namely those without exceedingly high degeneracies—are now covered in [6, 7] and in the present work. Accidental degeneracies due to fine-tuning of parameters should not lead to high degeneracies, but the quantitative effect of symmetries on level and gap degeneracies is not clear to the present authors. In order to better understand the occurrence of degeneracies, it appears indispensable to study specific examples. The harmonic oscillator would be one which is still not admissible (as the degeneracy of energy gaps is too large), but the hope that other relevant examples will be ‘tame’ enough seems reasonable.

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